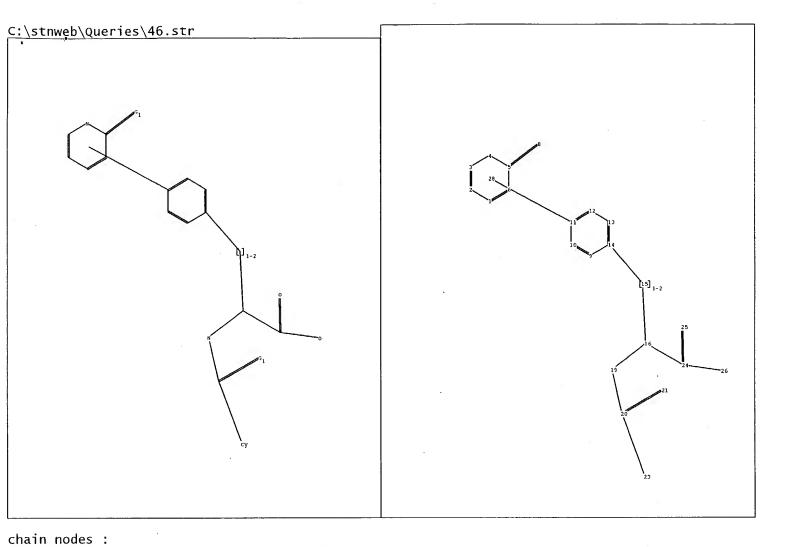


```
8 15 16 19 20 21 23 24 25 26
ring nodes:
    1 2 3 4 5 6 9 10 11 12 13 14
chain bonds:
    5-8 14-15 15-16 16-19 16-24 19-20 20-21 20-23 24-26 24-25
ring bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14
exact/norm bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 5-8 16-19 19-20 20-21 20-23 24-26 24-25
exact bonds:
    14-15 15-16 16-24
normalized bonds:
    9-10 9-14 10-11 11-12 12-13 13-14
isolated ring systems:
    containing 1 : 9 :
```

G1:0,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS 23:Atom
24:CLASS 25:CLASS 26:CLASS 28:CLASS



8 15 16 19 20 21 23 24 25 26
ring nodes:
 1 2 3 4 5 6 9 10 11 12 13 14
chain bonds:
 5-8 14-15 15-16 16-19 16-24 19-20 20-21 20-23 24-26 24-25
ring bonds:
 1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14
exact/norm bonds:
 1-2 1-6 2-3 3-4 4-5 5-6 5-8 16-19 19-20 20-21 20-23 24-26 24-25
exact bonds:
 14-15 15-16 16-24
normalized bonds:
 9-10 9-14 10-11 11-12 12-13 13-14
isolated ring systems:
 containing 1 : 9 :

G1:0,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS 23:Atom
24:CLASS 25:CLASS 26:CLASS 28:CLASS

* * * *	* *	* *	* *	* Welcome to STN International * * * * * * * * *		
NEWS :	1			Web Page URLs for STN Seminar Schedule - N. America		
	2			"Ask CAS" for self-help around the clock		
		JAN	27	Source of Registration (SR) information in REGISTRY updated and searchable		
NEWS 4	<u>4</u> J	JAN	27	A new search aid, the Company Name Thesaurus, available in CA/CAplus		
NEWS !	<u>5</u> F	EB	05	German (DE) application and patent publication number format changes		
NEWS	6 M	1AR	03	MEDLINE and LMEDLINE reloaded		
		1AR		MEDLINE file segment of TOXCENTER reloaded		
-	_	IAR		FRANCEPAT now available on STN		
NEWS :	_ 9 M	IAR	29	Pharmaceutical Substances (PS) now available on STN		
NEWS 1		IAR	29	WPIFV now available on STN		
NEWS 1	_	1AR		New monthly current-awareness alert (SDI) frequency in RAPRA		
NEWS 1		APR		PROMT: New display field available		
NEWS 1		APR	26	IFIPAT/IFIUDB/IFICDB: New super search and display field available		
NEWS 1	4 <i>P</i>	APR	26	LITALERT now available on STN		
NEWS 1		APR	27	NLDB: New search and display fields available		
NEWS 1	 6 M	lay	10	PROUSDDR now available on STN		
NEWS 1	_	lay		PROUSDDR: One FREE connect hour, per account, in both May and June 2004		
NEWS 1	8 M	lay	12	EXTEND option available in structure searching		
NEWS 1		lay		Polymer links for the POLYLINK command completed in REGISTRY		
NEWS 2	_	lay		FRFULL now available on STN		
NEWS 2		1ay		STN User Update to be held June 7 and June 8 at the SLA 2004		
NEWS 2	2 M	⁄lay	27	Conference New UPM (Update Code Maximum) field for more efficient patent		
		1		SDIs in CAplus		
NEWS 2	<u>3</u> N	⁄lay	27	CAplus super roles and document types searchable in REGISTRY		
NEWS 2	<u>4</u> N	1ay	27	Explore APOLLIT with free connect time in June 2004		
NEWS E	XPRE	<u>ESS</u>	MAC	RCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT CINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), D CURRENT DISCOVER FILE IS DATED 26 APRIL 2004		
MEMO II	OUDC	,		N Operating Hours Plus Help Desk Availability		
NEWS H				neral Internet Information		
NEWS L		-		lcome Banner and News Items		
NEWS P				cect Dial and Telecommunication Network Access to STN		
NEWS W		_		World Wide Web Site (general information)		
Enter Na specifie				ed by the item number or name to see news on that		
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research. Use for software development or design or implementation						

research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* \* STN Columbus

FILE 'HOME' ENTERED AT 17:36:03 ON 16 JUN 2004

=> file reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FILE 'REGISTRY' ENTERED AT 17:36:09 ON 16 JUN 2004
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STRUCTURE FILE UPDATES: 15 JUN 2004 HIGHEST RN 693773-36-3 DICTIONARY FILE UPDATES: 15 JUN 2004 HIGHEST RN 693773-36-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See <u>HELP CROSSOVER</u> for details.

Experimental and calculated property data are now available. For more information enter <a href="HELP PROP">HELP PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">http://www.cas.org/ONLINE/DBSS/registryss.html</a>

=> L1 STRUCTURE UPLOADED

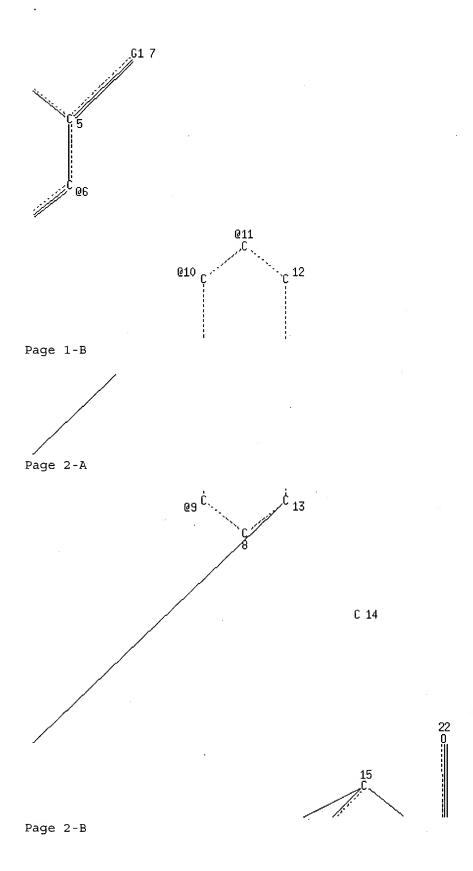
=> 1 1 IS NOT A RECOGNIZED COMMAND

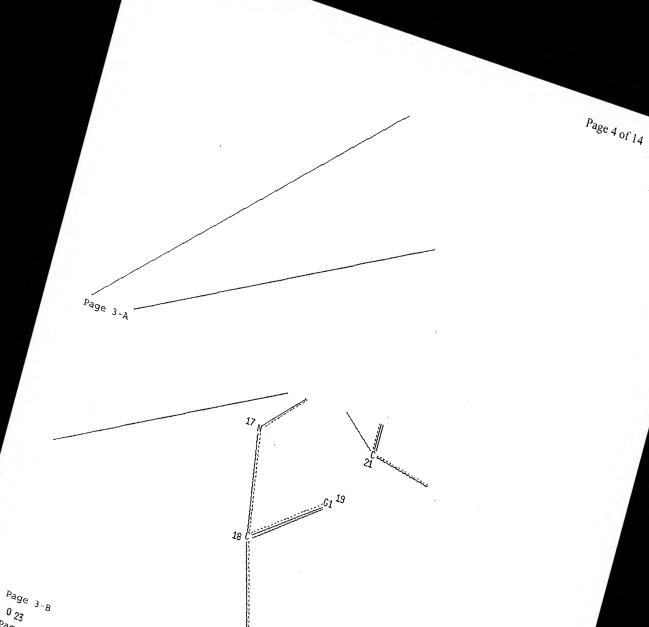
The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

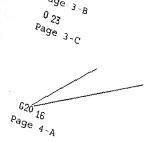
=> d 11 L1 HAS NO ANSWERS L1 STR 0 24 \$ 25

3 0--------

Page 1-A







http://stnweb.cas.org/cgi-bin/sdcgi?SID=170027-1564795372-200&APP=stnweb&

```
Page 4-B
VAR G1=24/25
REP G20=(1-2) 14-13 14-15
VPA 6-9/10/11 S
NODE ATTRIBUTES:
NSPEC
        IS R
                   AT
                        1
NSPEC
        IS R
                   AT
NSPEC
        IS R
                  AT
NSPEC
        IS R
                  AT
NSPEC
        IS R
                   AT
        IS R
NSPEC
                  AT
NSPEC
        IS C
                   AT
NSPEC
        IS R
                   AT
                        8
NSPEC
       IS R
                  AT
                        9
NSPEC
       IS R
                  AT
                     10
NSPEC
        IS R
                  AT
                      11
NSPEC
        IS R
                  AT
                     12
        IS R
NSPEC
                  AT
                      13
NSPEC
        IS C
                  \mathbf{AT}
                       14
NSPEC
        IS C
                  AT
                       15
NSPEC
        IS C
                  AT
                       16
NSPEC
        IS C
                  AT
                      17
NSPEC
       IS C
                  \mathtt{AT}
                      18
NSPEC
        IS C
                  AT
                      19
NSPEC
        IS C
                   AT
                       20
NSPEC
        IS C
                   AT
                       21
NSPEC
        IS C
                   AT
                       22
NSPEC
        IS C
                   AΤ
DEFAULT MLEVEL IS ATOM
                     14 15 17 18 21 22 23 24 25
MLEVEL IS CLASS AT
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 25
STEREO ATTRIBUTES: NONE
=> s 11
SAMPLE SEARCH INITIATED 17:40:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -
                                      355 TO ITERATE
100.0% PROCESSED
                      355 ITERATIONS
                                                                  2 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE
                                 **COMPLETE**
                                 **COMPLETE**
                         BATCH
PROJECTED ITERATIONS:
                               5970 TO
                                            8230
PROJECTED ANSWERS:
                                  2 TO
              2 SEA SSS SAM L1
L2
```

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

=> s 11 full

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y FULL SEARCH INITIATED 17:40:20 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 7084 TO ITERATE

100.0% PROCESSED 7084 ITERATIONS

42 ANSWERS

SEARCH TIME: 00.00.01

L3 42 SEA

42 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

157.94 158.15

FILE 'HCAPLUS' ENTERED AT 17:40:24 ON 16 JUN 2004
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FILE COVERS 1907 - 16 Jun 2004 VOL 140 ISS 25 FILE LAST UPDATED: 15 Jun 2004 (20040615/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12

L4 1 L2

=> d 14, ibib abs fhitstr, 1

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER:

2001:435046 HCAPLUS

DOCUMENT NUMBER:

135:33647

TITLE: INVENTOR(S): Preparation of pyridinyl phenylalanine derivatives Kaplan, Gerald Lewis; Sidduri, Achyutharao; Tilley,

Jefferson Wright

PATENT ASSIGNEE(S): SOURCE: F. Hoffmann-La Roche A.-G., Switz.

PCT Int. Appl., 97 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

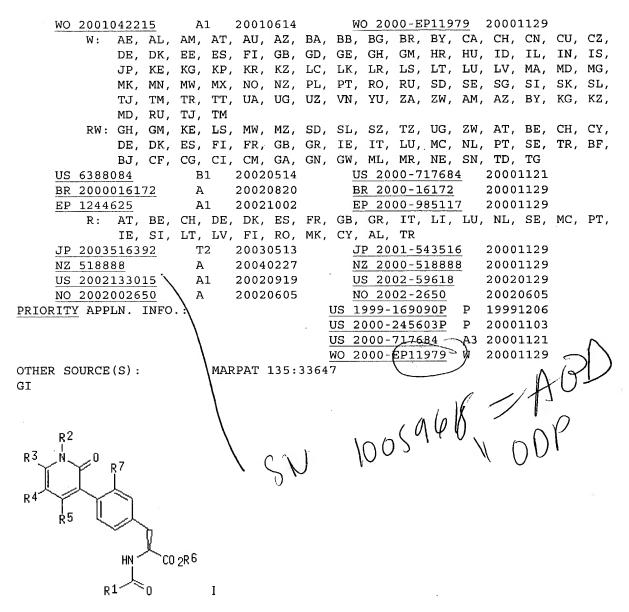
LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE



AB Pyridinyl phenylalanine derivs. I (R1 = substituted aryl, substituted 5 or 6 membered heteroarom. ring contg. N, O and S bonded via a carbon atom to the amide carbonyl, 3-7 membered ring substituted with alkyl, alkenyl, fluorinealkenyl, arylalkyl, heteroarylalkyl, azidoalkyl, cyanoalkyl, hydroxyalkyl, alkyl sulfonyl, alkyl sulfinyl; R2 = H, (un)substituted alkyl, aryl, or arylalkyl; R3 = H, halogen, alkyl, trifluoromethyl, or aryl; R4 = H, halogen, alkyl, or aryl; R5 = H, alkyl, alkoxy, trifluoromethyl, or aryl; R6 = H, alkyl, alkylcarbonyloxy, substituted aminoalkyl, substituted heterocyclylalkyl; R7 = H, Cl, alkoxy, or alkyl) were prepd. as inhibitors of the binding of VCAM-1 to VLA-4 and are useful in treating chronic inflammatory diseases. Thus, N-[(2-chloro-6methylphenyl)carbonyl]-4-(5-chloro-1-methyl-2-oxo-3-pyridinyl)-Lphenylalanine (II) was prepd. from N-[(1,1-dimethylethoxy)carbonyl]-4-iodo-L-phenylalanine Me ester in 5 steps via palladium catalyzed reaction with 3-bromo-5-chloro-1-methyl-2-pyridinone and coupling with 2-chloro-6-methylbenzoic acid. II showed antiinflammatory activity in vitro in the VCAM/VLA-4 screening assay (IC50 < 1 nM).

## IT 343981-14-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of pyridinyl phenylalanine derivs. as anti-inflammatory agents)

RN 343981-14-6 HCAPLUS

CN L-Phenylalanine, 4-[5-chloro-1,2-dihydro-2-oxo-1-(phenylmethyl)-3-pyridinyl]-N-[[1-(2-methoxyethyl)cyclopentyl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

3

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

9.48
167.63

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE
-0.69
-0.69

FILE 'CAOLD' ENTERED AT 17:41:40 ON 16 JUN 2004
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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter  $\underline{\text{HELP FIRST}}$  for more information.

## => d his

(FILE 'HOME' ENTERED AT 17:36:03 ON 16 JUN 2004)

FILE 'REGISTRY' ENTERED AT 17:36:09 ON 16 JUN 2004

L1 STRUCTURE UPLOADED

L2 2 S L1

L3 42 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 17:40:24 ON 16 JUN 2004 L4 1 S L2

FILE 'CAOLD' ENTERED AT 17:41:40 ON 16 JUN 2004

=> s 13

L5 0 L3

=> file reg

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
0.42 168.05

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE 0.00 -0.69

FILE 'REGISTRY' ENTERED AT 17:41:45 ON 16 JUN 2004
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STRUCTURE FILE UPDATES: 15 JUN 2004 HIGHEST RN 693773-36-3 DICTIONARY FILE UPDATES: 15 JUN 2004 HIGHEST RN 693773-36-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter <a href="http://example.com/HELP\_PROP">HELP\_PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">http://www.cas.org/ONLINE/DBSS/registryss.html</a>

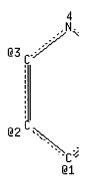
=> L6 STRUC

STRUCTURE UPLOADED

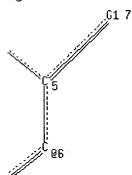
=> 16

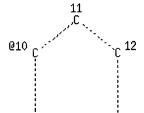
L6 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d 16 L6 HAS NO ANSWERS L6 STR



Page 1-A

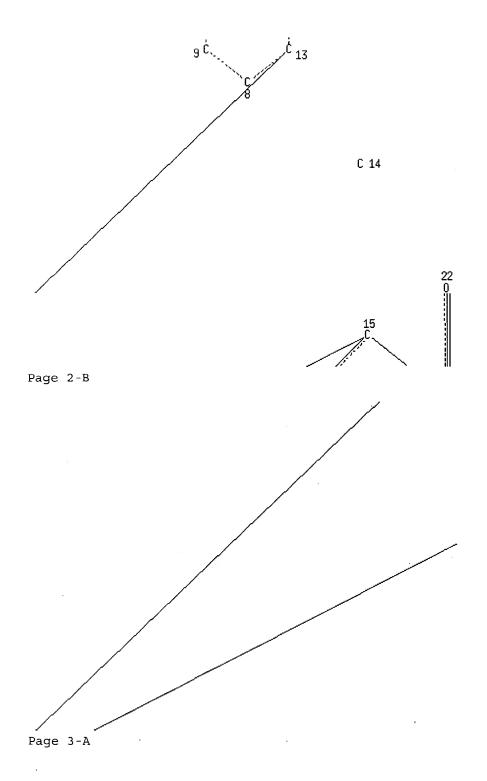


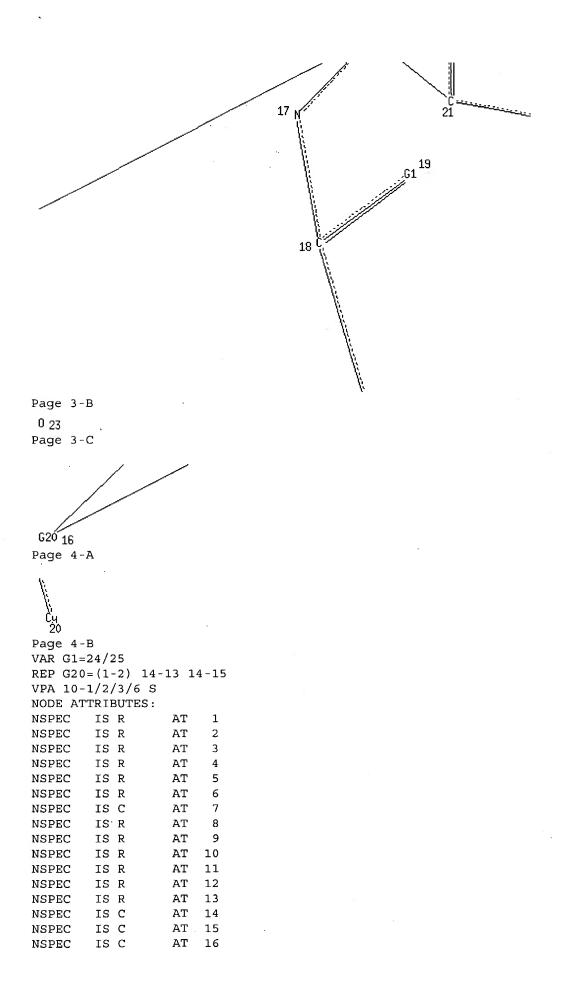


Page 1-B



Page 2-A





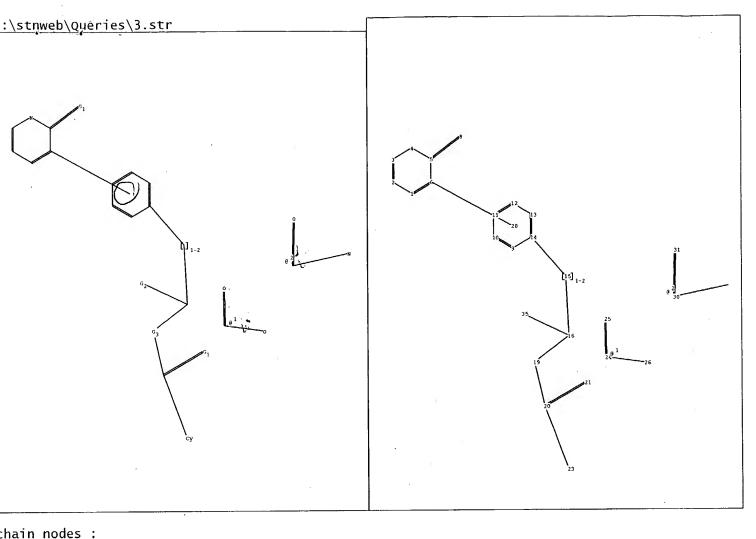
```
NSPEC
      IS C
                 AT 17
      IS C
NSPEC
                 AT
                     18
     IS C
                AT 19
NSPEC
NSPEC IS C
                 AT 20
NSPEC IS C
                 AT 21
NSPEC
     IS C
                 AT 22
NSPEC
      IS C
                 AT 23
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 14 15 17 18 21 22 23 24 25
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 25
STEREO ATTRIBUTES: NONE
=> s 16
SAMPLE SEARCH INITIATED 17:42:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 355 TO ITERATE
100.0% PROCESSED
                  355 ITERATIONS
                                                              2 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                       BATCH **COMPLETE**
PROJECTED ITERATIONS:
                             5970 TO 8230
PROJECTED ANSWERS:
                               2 TO
                                         124
L7
             2 SEA SSS SAM L6
=> s 16 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 17:42:47 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 7084 TO ITERATE
100.0% PROCESSED
                 7084 ITERATIONS
                                                             42 ANSWERS
SEARCH TIME: 00.00.01
           42 SEA SSS FUL L6
L8
=> d his
     (FILE 'HOME' ENTERED AT 17:36:03 ON 16 JUN 2004)
    FILE 'REGISTRY' ENTERED AT 17:36:09 ON 16 JUN 2004
               STRUCTURE UPLOADED
L1
L2
             2 S L1
L3
            42 S L1 FULL
     FILE 'HCAPLUS' ENTERED AT 17:40:24 ON 16 JUN 2004
L4
             1 S L2
     FILE 'CAOLD' ENTERED AT 17:41:40 ON 16 JUN 2004
L5
             0 S L3
    FILE 'REGISTRY' ENTERED AT 17:41:45 ON 16 JUN 2004
               STRUCTURE UPLOADED
L6
```

L7 2 S L6 L8 42 S L6 FULL

=> s 18 not 13

L9 0 L8 NOT L3

=>



G3:0,N

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS 23:Atom
24:CLASS 25:CLASS 26:CLASS 28:CLASS 30:CLASS 31:CLASS 32:CLASS 35:CLASS

G1:0,S

G2:[\*1],[\*2]

*	* *	* *	* *	* *	* Welcome to STN International * * * * * * * * *	
N	EWS	1			Web Page URLs for STN Seminar Schedule - N. America	
*****	EWS	2			"Ask CAS" for self-help around the clock	
N	EWS	3	JAN	27	Source of Registration (SR) information in REGISTRY updated	
	-				and searchable	
N	EWS	4	JAN	27	A new search aid, the Company Name Thesaurus, available in	
					CA/CAplus	
N	EWS	_5	FEB	05	German (DE) application and patent publication number format	
		_			changes	
	EWS	6	MAR		MEDLINE and LMEDLINE reloaded	
· man	EWS	7	MAR		MEDLINE file segment of TOXCENTER reloaded	
	EWS		MAR		FRANCEPAT now available on STN	
		9	MAR MAR		Pharmaceutical Substances (PS) now available on STN WPIFV now available on STN	
_	EWS		MAR		New monthly current-awareness alert (SDI) frequency in RAPRA	
	EWS EWS		APR		PROMT: New display field available	
_	EWS				IFIPAT/IFIUDB/IFICDB: New super search and display field	
14	<u> </u>		ALK	20	available	
N	EWS	14	APR	26	LITALERT now available on STN	
	EWS		APR		NLDB: New search and display fields available	
	EWS		May		PROUSDDR now available on STN	
	EWS		May		PROUSDDR: One FREE connect hour, per account, in both May	
			_		and June 2004	
N	EWS	18	May	12	EXTEND option available in structure searching	
N	EWS	19	May	12	Polymer links for the POLYLINK command completed in REGISTRY	
	EWS		May	17	FRFULL now available on STN	
N	EWS	21	May	27	STN User Update to be held June 7 and June 8 at the SLA 2004	
					Conference	
$\overline{\mathbf{N}}$	EWS	22	May	27	New UPM (Update Code Maximum) field for more efficient patent	
					SDIs in CAplus	
	EWS		May		CAplus super roles and document types searchable in REGISTRY	
N	EWS	24	May	27	Explore APOLLIT with free connect time in June 2004	
N	EWS	ביע דינ	סשפפ	MΛΤ	RCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT	
TA	EWO	EXFI	CEGG		CINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),	
					CURRENT DISCOVER FILE IS DATED 26 APRIL 2004	
N	EWS	HOUE	RS		V Operating Hours Plus Help Desk Availability	
			neral Internet Information			
			clome Banner and News Items			
		Dia	rect Dial and Telecommunication Network Access to STN			
		CAS	S World Wide Web Site (general information)			
Enter NEWS followed by the item number or name to see news on that						
specific topic.						

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FILE 'HOME' ENTERED AT 18:06:15 ON 16 JUN 2004

=> file reg COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FILE 'REGISTRY' ENTERED AT 18:06:22 ON 16 JUN 2004
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STRUCTURE FILE UPDATES: 15 JUN 2004 HIGHEST RN 693773-36-3 DICTIONARY FILE UPDATES: 15 JUN 2004 HIGHEST RN 693773-36-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Experimental and calculated property data are now available. For more information enter <a href="HELP PROP">HELP PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">http://www.cas.org/ONLINE/DBSS/registryss.html</a>

=> L1

STRUCTURE UPLOADED

=> 11

L1 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> d 11

L1 HAS NO ANSWERS

L1 STR

=> s 11

SAMPLE SEARCH INITIATED 18:08:48 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5368 TO ITERATE

18.6% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

PROJECTED ITERATIONS: BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 102968 TO 111752

PROJECTED ITERATIONS: 102968 TO 11175: PROJECTED ANSWERS: 1 TO 240

L2 1 SEA SSS SAM L1

=> s 11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 18:08:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 108719 TO ITERATE

100.0% PROCESSED 108719 ITERATIONS 42 ANSWERS SEARCH TIME: 00.00.04

1 ANSWERS

T.3 42 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

157.10 157.31

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FILE COVERS 1907 - 16 Jun 2004 VOL 140 ISS 25 FILE LAST UPDATED: 15 Jun 2004 (20040615/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13/thu

2 L3

599383 THU/RL

L4

1 L3/THU

(L3 (L) THU/RL)

=> d 14, ibib abs fhitstr, 1

ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

References Text ACCESSION NUMBER:

2001:435046 HCAPLUS

DOCUMENT NUMBER:

135:33647

TITLE: INVENTOR(S): Preparation of pyridinyl phenylalanine derivatives Kaplan, Gerald Lewis; Sidduri, Achyutharao; Tilley,

Jefferson Wright

PATENT ASSIGNEE(S):

F. Hoffmann-La Roche A.-G., Switz.

SOURCE:

PCT Int. Appl., 97 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		-,		
WO 2001042215	A1	20010614	WO 2000-EP11979	20001129

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,

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JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,
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             TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,
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PRIORITY APPLN. INFO .:
                                         US 2000-245603P P
                                                             20001103
                                         US 2000-717684 A3 20001121
                                         WO 2000 EP11979
                                                          W
                                                             20001129
                         MARPAT 135:33647____
OTHER SOURCE(S):
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GI

I

Pyridinyl phenylalanine derivs. I (R1 = substituted aryl, substituted 5 or AB 6 membered heteroarom. ring contg. N, O and S bonded via a carbon atom to the amide carbonyl, 3-7 membered ring substituted with alkyl, alkenyl, fluorinealkenyl, arylalkyl, heteroarylalkyl, azidoalkyl, cyanoalkyl, hydroxyalkyl, alkyl sulfonyl, alkyl sulfinyl; R2 = H, (un)substituted alkyl, aryl, or arylalkyl; R3 = H, halogen, alkyl, trifluoromethyl, or aryl; R4 = H, halogen, alkyl, or aryl; R5 = H, alkyl, alkoxy, trifluoromethyl, or aryl; R6 = H, alkyl, alkylcarbonyloxy, substituted aminoalkyl, substituted heterocyclylalkyl; R7 = H, Cl, alkoxy, or alkyl) were prepd. as inhibitors of the binding of VCAM-1 to VLA-4 and are useful in treating chronic inflammatory diseases. Thus, N-[(2-chloro-6methylphenyl)carbonyl]-4-(5-chloro-1-methyl-2-oxo-3-pyridinyl)-Lphenylalanine (II) was prepd. from N-[(1,1-dimethylethoxy)carbonyl]-4-iodo-L-phenylalanine Me ester in 5 steps via palladium catalyzed reaction with 3-bromo-5-chloro-1-methyl-2-pyridinone and coupling with 2-chloro-6-methylbenzoic acid. II showed antiinflammatory activity in vitro in the VCAM/VLA-4 screening assay (IC50 < 1 nM).

IT 343981-05-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of pyridinyl phenylalanine derivs. as anti-inflammatory agents)

RN 343981-05-5 HCAPLUS

CN L-Phenylalanine, 4-(5-chloro-1,2-dihydro-1-methyl-2-oxo-3-pyridinyl)-N-(2-chloro-6-methylbenzoyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.12	164.43
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.69	-0.69

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter  $\underline{\text{HELP FIRST}}$  for more information.

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(FILE 'HOME' ENTERED AT 18:06:15 ON 16 JUN 2004)

FILE 'REGISTRY' ENTERED AT 18:06:22 ON 16 JUN 2004

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 42 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 18:09:04 ON 16 JUN 2004

L4 1 S L3/THU

FILE 'CAOLD' ENTERED AT 18:09:34 ON 16 JUN 2004

=> s 13

L5 0 L3

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